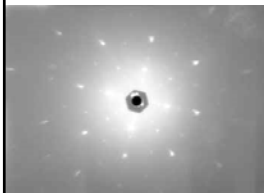


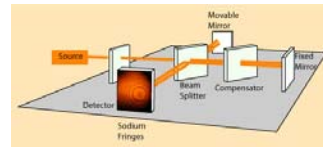
# Phys 446: Solid State Physics / Optical Properties

Fall 2015



Lecture 2

Andrei Sirenko, NJIT



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## Solid State Physics

### Lecture 2

(Ch. 2.1-2.3, 2.6-2.7)

Last week:

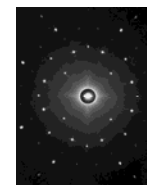
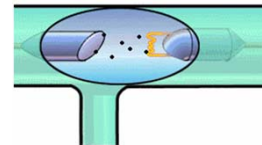
- Crystals,
- Crystal Lattice,
- Reciprocal Lattice

Today:

- Types of bonds in crystals

Diffraction from crystals

- Importance of the *reciprocal lattice* concept



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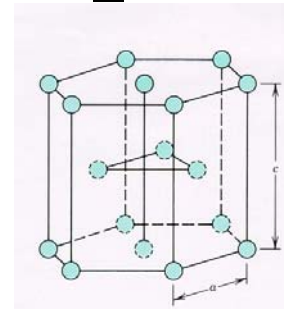
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### (3) The Hexagonal Closed-packed (HCP) structure

Be, Sc, Te, Co, Zn, Y, Zr, Tc, Ru, Gd, Tb, Py, Ho, Er, Tm, Lu, Hf, Re, Os, Ti

- The HCP structure is made up of stacking spheres in a ABABAB... configuration
- The HCP structure has the primitive cell of the hexagonal lattice, with a basis of two identical atoms
- Atom positions: 000,  $2/3 \ 1/3 \ 1/2$  (remember, the unit axes are not all perpendicular)
- The number of nearest-neighbours is 12
- The ideal ratio of  $c/a$  for this packing is  $(8/3)^{1/2} = 1.633$



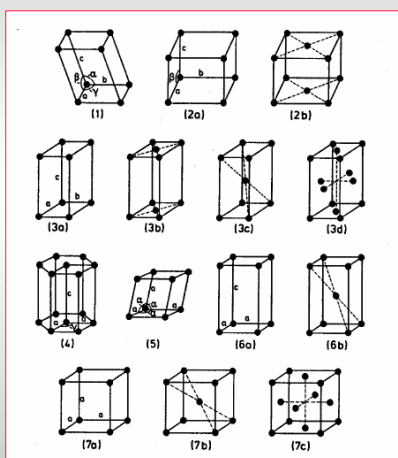
Rotated three times

Conventional HCP unit cell

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### Crystal Lattice



**14 Bravais Lattices which can be assigned to 7 different Crystal Systems**

- |                         |                   |   |
|-------------------------|-------------------|---|
| <b>(1) triclinic</b>    | $a \neq b \neq c$ | $\alpha \neq \beta \neq \gamma$                 |
| <b>(2) monoclinic</b>   | $a \neq b \neq c$ | $\alpha = \gamma = 90^\circ \neq \beta$         |
| a) primitive            |                   |   |
| b) base centered        |                   |   |
| <b>(3) orthorhombic</b> | $a \neq b \neq c$ | $\alpha = \beta = \gamma = 90^\circ$            |
| a) primitive            |                   |   |
| b) base centered        |                   |   |
| c) space centered       |                   |   |
| d) face centered        |                   |   |
| <b>(4) hexagonal</b>    | $a = b \neq c$    | $\alpha = \beta = 90^\circ, \gamma = 120^\circ$ |
| <b>(5) trigonal</b>     | $a = b = c$       | $\alpha = \beta = \gamma \neq 90^\circ$         |
| <b>(6) tetragonal</b>   | $a = b \neq c$    | $\alpha = \beta = \gamma = 90^\circ$            |
| a) primitive            |                   |   |
| b) space centered       |                   |   |
| <b>(7) cubic</b>        | $a = b = c$       | $\alpha = \beta = \gamma = 90^\circ$            |
| a) primitive            |                   |   |
| b) space centered       |                   |   |
| c) face centered        |                   |   |

[http://www.matter.org.uk/diffraction/geometry/reciprocal\\_lattice\\_exercises.htm](http://www.matter.org.uk/diffraction/geometry/reciprocal_lattice_exercises.htm)

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## Reciprocal Lattice

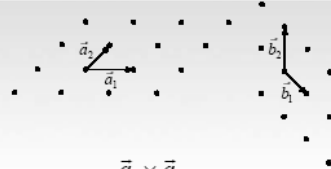
crystal lattice point:  $\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$

reciprocal lattice point:  $\vec{G} = h_1\vec{b}_1 + h_2\vec{b}_2 + h_3\vec{b}_3$

primitive translations of the reciprocal lattice:

$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3} \quad \vec{b}_2 = 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3} \quad \vec{b}_3 = 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3}$$

properties:  $\vec{a}_i \cdot \vec{b}_k = 2\pi\delta_{ik}$  or  $\vec{R} \cdot \vec{G} = m2\pi$



fundamental property of a crystal lattice:  
translation invariance of electron- / scattering-density:

$$\rho(\vec{r}) = \rho(\vec{r} + \vec{R})$$

$$\rho(\vec{r}) = \sum_{\vec{G}} \rho_{\vec{G}} e^{i\vec{G}\cdot\vec{r}} \quad \text{with} \quad \rho(\vec{r} + \vec{R}) = \sum_{\vec{G}} \rho_{\vec{G}} e^{i(\vec{G}\cdot\vec{r} + \vec{G}\cdot\vec{R})} = \sum_{\vec{G}} \rho_{\vec{G}} e^{i\vec{G}\cdot\vec{r}} = \rho(\vec{r})$$

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## Some examples of reciprocal lattices

### 1. Reciprocal lattice to simple cubic lattice

$$\mathbf{a}_1 = a\mathbf{x}, \quad \mathbf{a}_2 = a\mathbf{y}, \quad \mathbf{a}_3 = a\mathbf{z} \quad V = \mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3) = a^3 \Rightarrow$$

$$\mathbf{b}_1 = (2\pi/a)\mathbf{x}, \quad \mathbf{b}_2 = (2\pi/a)\mathbf{y}, \quad \mathbf{b}_3 = (2\pi/a)\mathbf{z} \quad \Rightarrow$$

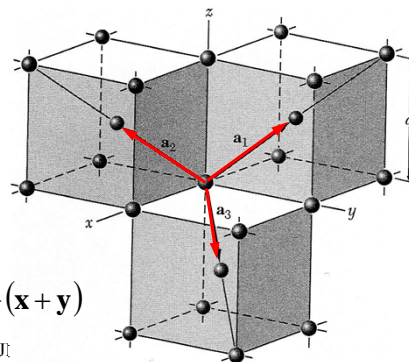
reciprocal lattice is also cubic with lattice constant  $2\pi/a$

### 2. Reciprocal lattice to bcc lattice

$$\mathbf{a}_1 = \frac{1}{2}a(-\mathbf{x} + \mathbf{y} + \mathbf{z}) \quad \mathbf{a}_2 = \frac{1}{2}a(\mathbf{x} - \mathbf{y} + \mathbf{z})$$

$$\mathbf{a}_3 = \frac{1}{2}a(\mathbf{x} + \mathbf{y} - \mathbf{z}) \quad V = |\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3| = \frac{1}{2}a^3$$

$$\Rightarrow \mathbf{b}_1 = \frac{2\pi}{a}(\mathbf{y} + \mathbf{z}) \quad \mathbf{b}_2 = \frac{2\pi}{a}(\mathbf{x} + \mathbf{z}) \quad \mathbf{b}_3 = \frac{2\pi}{a}(\mathbf{x} + \mathbf{y})$$



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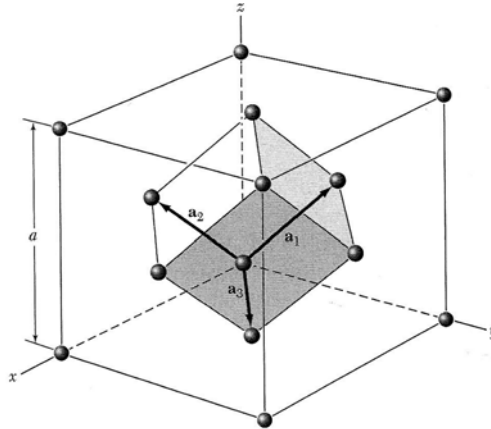
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got  $\mathbf{b}_1 = \frac{2\pi}{a}(\mathbf{y} + \mathbf{z})$

$\mathbf{b}_2 = \frac{2\pi}{a}(\mathbf{x} + \mathbf{z})$

$\mathbf{b}_3 = \frac{2\pi}{a}(\mathbf{x} + \mathbf{y})$

but these are primitive vectors of fcc lattice



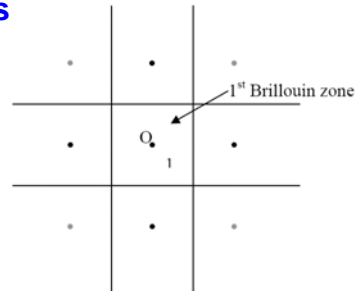
So, the reciprocal lattice to bcc is fcc.

Analogously, show that the reciprocal lattice to fcc is bcc

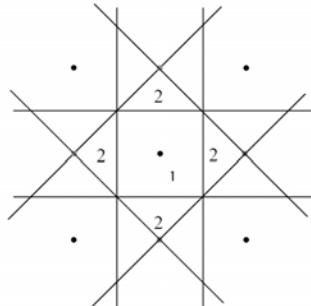
### Brillouin zones

Determine all the perpendicular bisecting planes in the reciprocal lattice

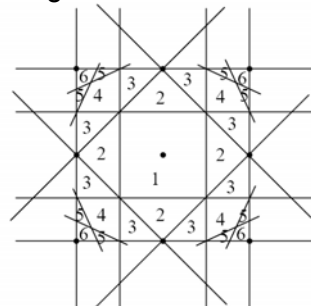
First Brillouin zone - the Wigner-Seitz cell of the reciprocal lattice



Second Brillouin zone:

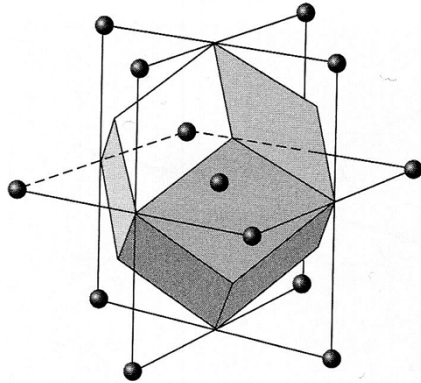


Higher Brillouin zones:

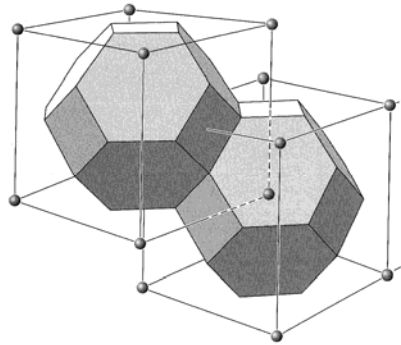


## Brillouin zones of cubic lattices

First BZ of a BCC lattice



First BZ of an FCC lattice



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## Summary

- ❖ Reciprocal lattice is defined by primitive vectors:

$$\mathbf{b}_1 = \frac{2\pi}{V} \mathbf{a}_2 \times \mathbf{a}_3, \quad \mathbf{b}_2 = \frac{2\pi}{V} \mathbf{a}_3 \times \mathbf{a}_1, \quad \mathbf{b}_3 = \frac{2\pi}{V} \mathbf{a}_1 \times \mathbf{a}_2$$

- ❖ A reciprocal lattice vector has the form  $\mathbf{G} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3$   
It is normal to (hkl) planes of direct lattice
- ❖ First Brillouin zone is the Wigner-Seitz primitive cell of the reciprocal lattice
- ❖ Simple cubic  $\rightarrow$  cube; bcc  $\rightarrow$  Rhombic dodecahedron;  
fcc  $\rightarrow$  truncated octahedron (figures on the previous slide)

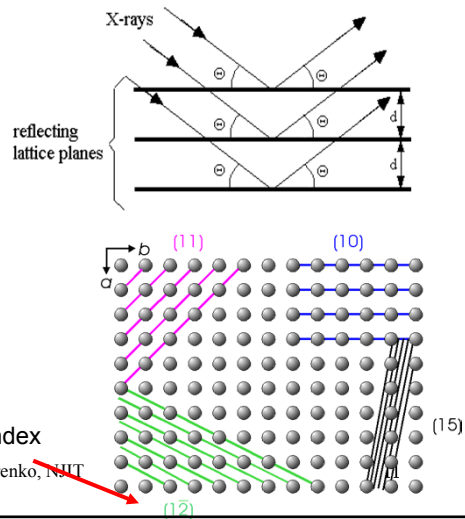
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# Indexing system for crystal planes

- Since crystal structures are obtained from diffraction experiments (in which particles diffract from planes of atoms), it is useful to develop a system for indexing lattice planes.
- We can use the lattice constants  $a_1, a_2, a_3$ , but it turns out to be more useful to use what are called Miller Indices.

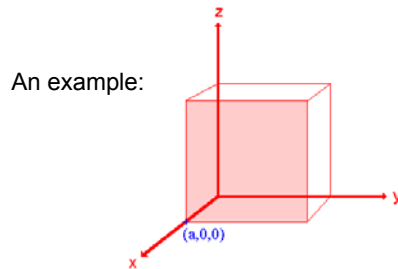


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# Rules for determining Miller Indices

- (1) Find the intercepts on the axes in terms of the lattice constants  $a_1, a_2, a_3$ .
- (2) Take the reciprocals of these numbers and then reduce to three integers having the same ratio, usually the smallest of the three integers. The result, listed as  $(hkl)$ , is called the index of the plane.



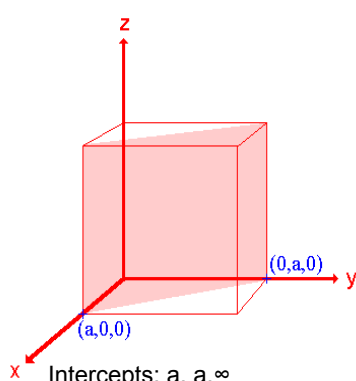
Intercepts:  $a, \infty, \infty$   
 Reciprocals:  $a/a, a/\infty, a/\infty$   
 $= 1, 0, 0$   
 Miller index for this plane :  $(1\ 0\ 0)$   
 (note: this is the normal vector for this plane)

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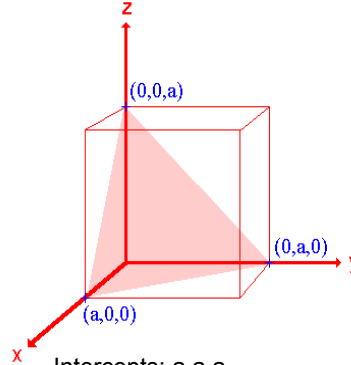
## Examples of Miller Indices



Intercepts:  $a, a, \infty$   
 Reciprocals:  $a/a, a/a, a/\infty$   
 $= 1, 1, 0$   
 Miller index for this plane :  $(1\ 1\ 0)$

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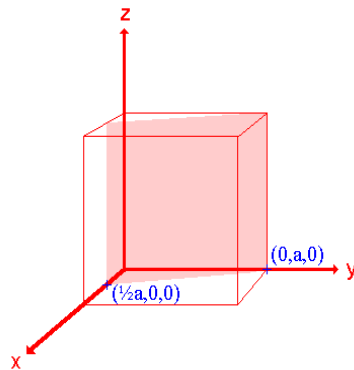
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Intercepts:  $a, a, a$   
 Reciprocals:  $a/a, a/a, a/a$   
 $= 1, 1, 1$   
 Miller index for this plane :  $(1\ 1\ 1)$

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## Examples of Miller Indices



Intercepts:  $1/2a, a, \infty$   
 Reciprocals:  $2a/a, a/a, a/\infty$   
 $= 2, 1, 0$   
 Miller index for this plane :  $(2\ 1\ 0)$

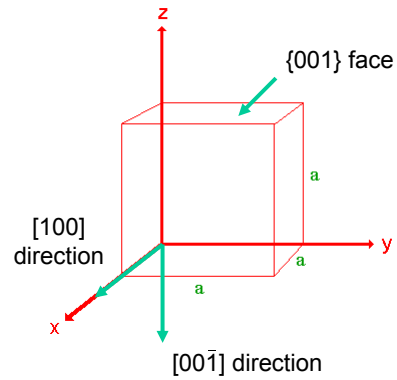
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## Notes on notation

- $(hkl)$  might mean a single plane, or a set of planes
- If a plane cuts a negative axis, we have minus signs in the  $(hkl)$  (ie.  $(h\bar{k}l)$ )
- Planes are denoted with curly brackets  $\{hkl\}$
- A set of faces are denoted  $\{hkl\}$
- The direction of a crystal (for example, along  $x$  for a cubic crystal) is denoted with  $[uvw]$  (ie. The  $[100]$  direction)
- In cubic crystals, the direction  $[hkl]$  is perpendicular to the plane  $(hkl)$  having the same indices, but this isn't necessarily true for other crystal systems



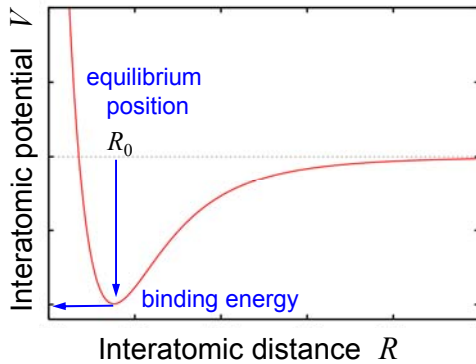
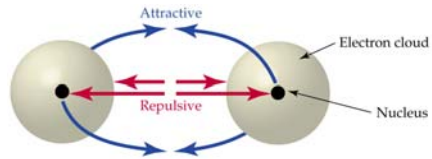
## Inter-atomic forces and types of bonds in solids.



## Interatomic forces

What holds a crystal together?

Attractive electrostatic interaction between electrons and nuclei – the force responsible for cohesion of solids



Force:

$$F(R) = -\frac{\partial V(R)}{\partial R}$$

$F(R) < 0$  for  $R > R_0$  :  
attraction

$F(R) > 0$  for  $R < R_0$  :  
repulsion

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## Types of bonding

### I. Ionic crystals

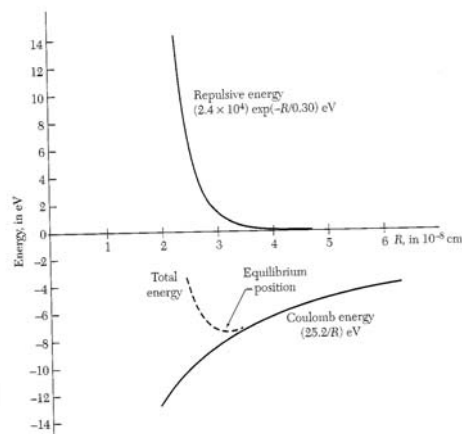
Usually involve atoms of strongly different electro-negativities (Example: alkali halides).

$$U(R) = -N \frac{\alpha e^2}{4\pi\epsilon_0 R} + N \frac{A}{R^n}$$

attractive  
(Coulomb)

repulsive

Ionic bond is strong  
(binding energy - few eV/pair)  
⇒ hardness, high melting T  
electrons are strongly localized  
⇒ insulators in solid form



KCl: energy per molecule vs  $R$   
(from Kittel)

Typical crystal structures: NaCl, CsCl

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## II. Covalent crystals

- Electron pair bond: usually one electron from each atom
- Electrons tend to be localized in part between the two atoms
- The spins of electrons in the bond are anti-parallel
- Gap between fully occupied and unoccupied states → dielectrics or semiconductors

Directionality of covalent bonds. Example: carbon

Hybridization.  $2s^2 2p^2 \rightarrow 2s 2p_x 2p_y 2p_z$ :  $sp^3$  tetrahedral configuration

Also possible  $sp^2$ :  $2s 2p_x 2p_y$  – planar (graphite, fullerenes)  
remaining  $p_z$ : interlayer  $\pi$ -bonding

Covalent polar bond (many compound semiconductors) – intermediate case between non-polar and ionic bond. Described by effective ionic charge or fractional ionic character (between 0 and 1: 0 for Si or diamond, 0.94 for NaCl). Covalent bond is also strong, binding energies of several eV per atom

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## III. Metals

- Most elements in periodic table
- High electrical and thermal conductivity
- High density
- Considerable mechanical strength, but plasticity

These properties can be explained considering the metallic type of bond

Example: alkali metals – single electron weakly bound to atom – easily delocalized.

In contrast to covalent bonding, electronic wave functions are very extended compared to interatomic distances. Why total energy is reduced ?

Partially occupied electronic bands – electrons can move freely

Group II metals – two  $s$  electrons – should be fully occupied...  
but overlapped with empty  $p$ -states

Transition metals:  $d$ -electrons are more localized – form covalent-like bonds;  $s$  and  $p$ -electrons again form a common band

Metals crystallize in closely packed structures (hcp, fcc, bcc)

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#### IV. Van der Waals bonds

Inert gases: outer electronic shells are full – no ionic or covalent forces

Weak interatomic forces due to quantum fluctuations of charge → arising dipole moments cause a weak attractive force

Can be described in the quantum-mechanical model of two linear oscillators (given in Kittel) → results in  $R^{-6}$  dependence of potential

Binding energy in order of 0.1 eV

Crystal structures are fcc (electronic distribution is spherical, atoms pack as closely as possible)

Van der Waals forces are also responsible for bonding in organic molecular crystals. Molecules are weakly bound; often form low-symmetry crystals

They also exist in covalent or ionic crystals, but negligible

#### V. Hydrogen bonds

Formed between two strongly electronegative atoms (F, O, N) via H

Example: ice

Binding energy is also ~0.1 eV

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#### Summary

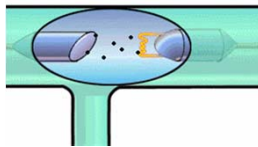
- ❖ Repulsive interaction between atoms is primarily due to electrostatic repulsion of overlapping charge distributions and Pauli principle
- ❖ Several types of attractive forces:
  - Ionic crystals – electrostatic forces between "+" and "-" ions
  - Covalent bond: overlap of charge distributions with antiparallel spin
  - Metals: reduction of kinetic energy of electrons in free state compared to the localized state of a single atom
  - Secondary forces (Van der Waals, hydrogen) become significant when the other bonds are impossible, e.g. in inert gases
- ❖ Physical properties are closely related to the type of bonding

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# DIFFRACTION



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## Diffraction of **waves** by crystal lattice

- Most methods for determining the atomic structure of crystals are based on scattering of particles/radiation.
- X-rays is one of the types of the radiation which can be used
- Other types include electrons and neutrons
- The wavelength of the radiation should be comparable to a typical interatomic distance of a few Å (1 Å = 10<sup>-10</sup> m)

$$E = h\nu = \frac{hc}{\lambda} \Rightarrow \lambda = \frac{hc}{E}$$

$$\lambda(\text{\AA}) = 12398/E(\text{eV}) \Rightarrow$$

few keV is suitable energy  
for  $\lambda = 1 \text{ \AA}$

- X-rays are scattered mostly by electronic shells of atoms in a solid. Nuclei are too heavy to respond.
- Reflectivity of x-rays  $\sim 10^{-3}$ - $10^{-5} \Rightarrow$  deep penetration into the solid  
 $\Rightarrow$  x-rays serve as a bulk probe

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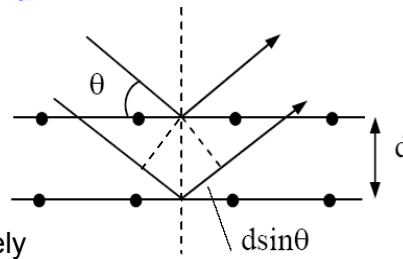
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## The Bragg Law

Conditions for a sharp peak in the intensity of the scattered radiation:

- 1) the x-rays should be specularly reflected by the atoms in one plane
- 2) the reflected rays from the successive planes interfere constructively



The path difference between the two x-rays:  $2d \cdot \sin\theta \Rightarrow$

the Bragg formula:  $2d \cdot \sin\theta = m\lambda$

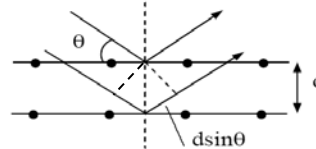
The model used to get the Bragg law are greatly oversimplified (but it works!).

- It says nothing about intensity and width of x-ray diffraction peaks
- neglects differences in scattering from different atoms
- assumes single atom in every lattice point
- neglects distribution of charge around atoms

## The Bragg Law and Diffraction grating

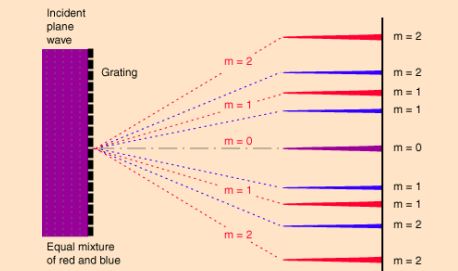
Compare Bragg Law

$$2d \cdot \sin\theta = m\lambda$$



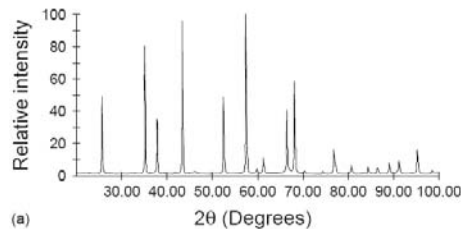
### Diffraction Grating

A diffraction grating is the tool of choice for separating the colors in incident light.



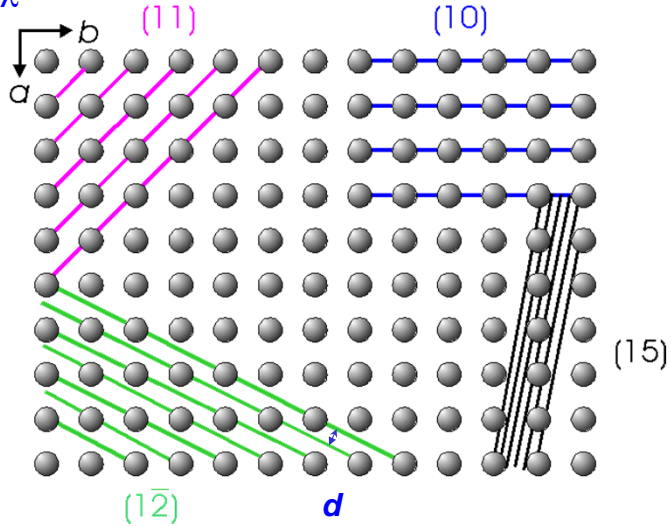
The condition for maximum intensity is the same as that for a double slit. However, angular separation of the maxima is generally much greater because the slit spacing is so small for a diffraction grating.

### X-ray Diffraction



### Meaning of $d$ for 2D

$$2d \cdot \sin\theta = m\lambda$$



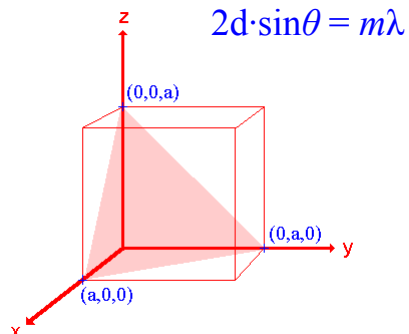
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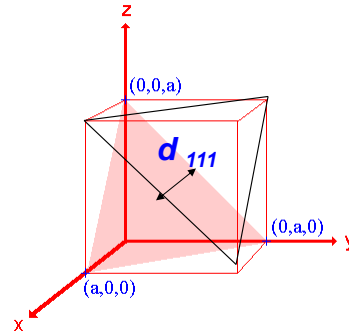
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### Meaning of $d$ for 3D

[http://www.desy.de/~luebbert/CrystalCalc\\_Cubic.htm](http://www.desy.de/~luebbert/CrystalCalc_Cubic.htm)



Intercepts:  $a, a, a$   
 Reciprocals:  $a/a, a/a, a/a$   
 $= 1, 1, 1$   
 Miller index for this plane : (1 1 1)



$$d_{hkl} = \frac{n}{\sqrt{\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}}}$$

$$d_{111} = \frac{n \cdot a}{\sqrt{3}} \approx 3.13 \text{ \AA} \text{ for Si with } a = 5.431 \text{ \AA}$$

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### Calculating the angle between two planes

For cubic crystals, the angle,  $\phi$  between two planes,  $(h_1 k_1 l_1)$  and  $(h_2 k_2 l_2)$  is given by:

$$\cos \phi = \frac{h_1 h_2 + k_1 k_2 + l_1 l_2}{\sqrt{h_1^2 + k_1^2 + l_1^2} \sqrt{h_2^2 + k_2^2 + l_2^2}}$$

#### Example:

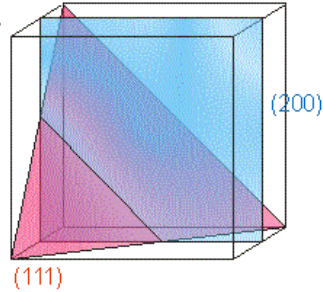
Calculate the angle between the (111) and (200) planes.

From the above,

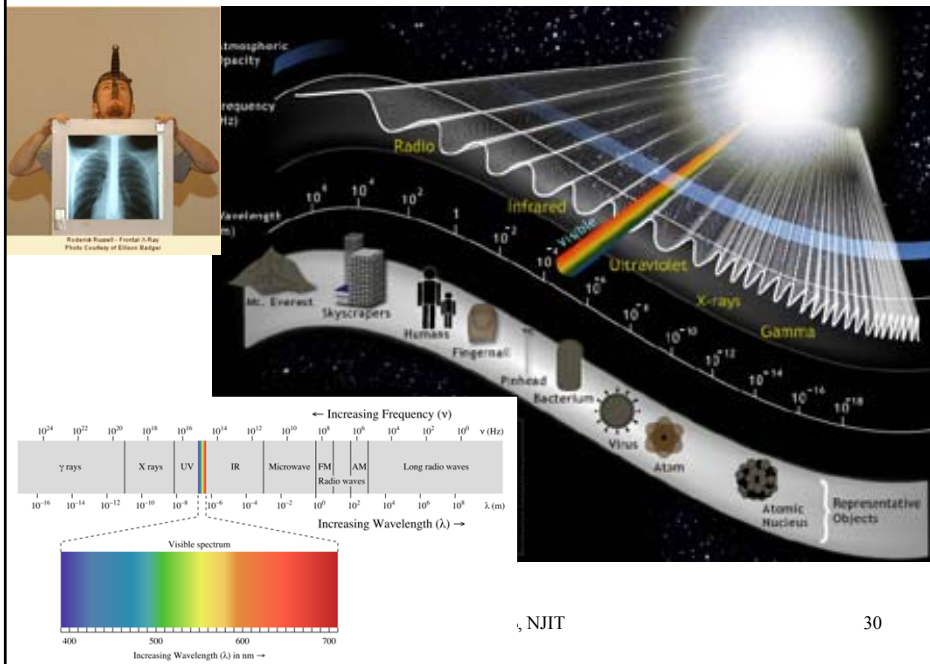
$$\cos \phi = \frac{(1 \times 2) + (1 \times 0) + (1 \times 0)}{\sqrt{1+1+1} \sqrt{4+0+0}}$$

$$\cos \phi = \frac{1}{\sqrt{3}}$$

which produces the result,  $\phi = 54.75^\circ$ .



### X-rays are EM waves



The most important information arises when the wavelength of the radiation is similar to, or smaller than, the size of the spacing between the objects being studied.

Electron-beam (3.7 pm for 100 keV)	Scatterers (spacings)	Radiation (typical dimension)
Light (520 nm for green)	Ink dots in newsprint (0.1 mm)	
X-ray (0.154 nm for Cu K $\alpha$ )	Raindrops (10 mm)	
Sound (1.26 m at middle C)	Row of parked cars (3 m)	
Thermal radiation (0.1 nm typical)	Precipitates in alloys (100 nm)	
	Atoms in crystals (0.1 nm)	

Reset Score

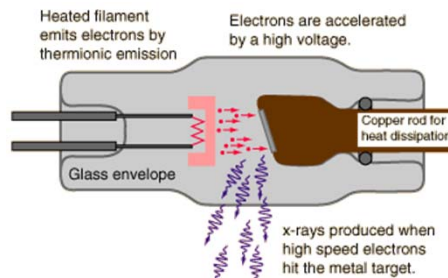
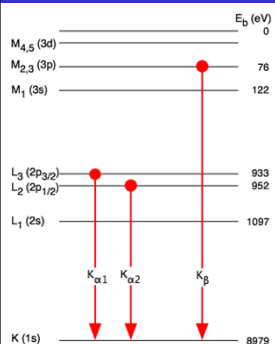
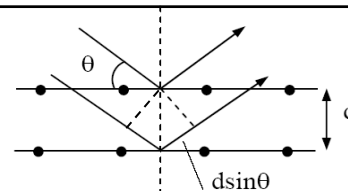
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### X-rays and X-ray tube

Bragg Law

$$2d \cdot \sin\theta = m\lambda$$

for  $m=1$   $2d > \lambda$



### X-ray tube

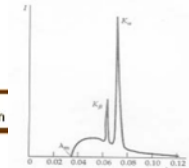
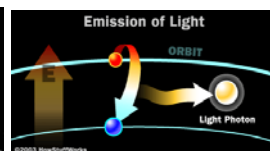
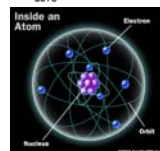


Figure 37-19 X-ray spectrum of molybdenum. The sharp peaks labeled  $K_{\alpha}$  and  $K_{\beta}$  are characteristic of the element. The cutoff wavelength  $\lambda_{cut}$  is independent of the target element and is related to the voltage  $V$  of the x-ray tube by  $\lambda_{cut} = hc/eV$ .

### Electronic transitions



X-ray K-series spectral line wavelengths (nm) for some common target materials.<sup>[5]</sup>

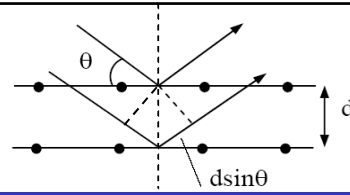
Target	K $\beta_1$	K $\beta_2$	K $\alpha_1$	K $\alpha_2$
Fe	0.17566	0.17442	0.193604	0.193998
Ni	0.15001	0.14886	0.165791	0.166175
Cu	0.139222	0.138109	0.154056	0.154439
Zr	0.070173	0.068993	0.078593	0.079015
Mo	0.063229	0.062099	0.070930	0.071359



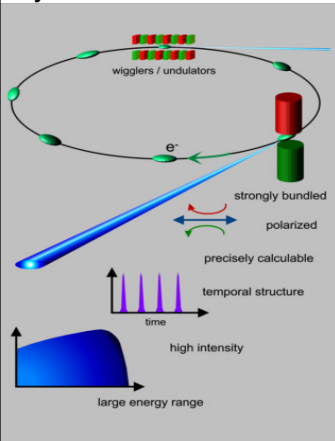
## X-rays and Synchrotrons

Bragg Law

$$2d \cdot \sin\theta = m\lambda$$

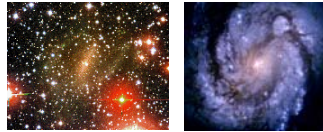


### Synchrotron radiation

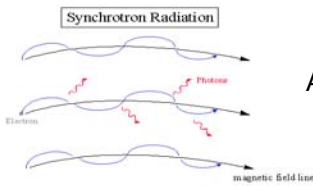


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### Natural Synchrotron Radiation



Stars and Galaxies



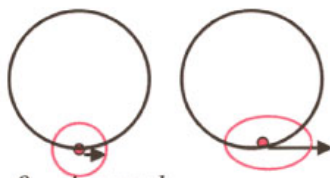
Accelerating electron emits light

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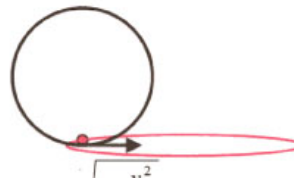
## SYNCHROTRON RADIATION

$v \ll c$



$\theta = 4\pi \text{ srad}$

$v \approx 0.99999999 c$



$\theta \approx \sqrt{1 - \frac{v^2}{c^2}} \approx 0.001 \text{ srad}$

Synchrotron Radiation produced by relativistic electrons in accelerators (since 1947)

### NLSL:

- 50 m circumference,
- Current = 1 A,
- $f=6$  MHz,
- $E=800\text{MeV}$  (restmass energy  $E_0 \approx 0.5\text{MeV}$ )
- $I \propto \lambda^{-7/3}$

- **Synchrotron Radiation from a storage ring is the most bright manmade source of white light**
- **Useful for materials studies from Far Infrared and UV to X-ray**

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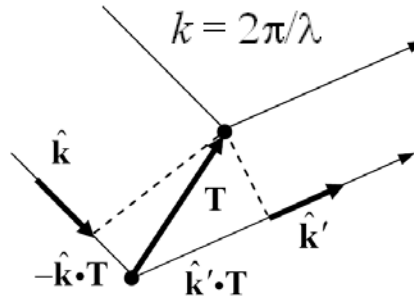
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## Diffraction condition and reciprocal lattice

Von Laue approach:

- crystal is composed of identical atoms placed at the lattice sites  $\mathbf{T}$
- each atom can reradiate the incident radiation in all directions.
- Sharp peaks are observed only in the directions for which the x-rays scattered from all lattice points interfere constructively.



Consider two scatterers separated by a lattice vector  $\mathbf{T}$ . Incident x-rays: wavelength  $\lambda$ , wavevector  $\mathbf{k}$ ;  $|\mathbf{k}| = k = 2\pi/\lambda$ ; Assume *elastic* scattering: scattered x-rays have same energy (same  $\lambda$ )  $\Rightarrow$  wavevector  $\mathbf{k}'$  has the same magnitude  $|\mathbf{k}'| = k = 2\pi/\lambda$

Condition of constructive interference:  $(\mathbf{k}' - \mathbf{k}) \cdot \mathbf{T} = 2\pi m$

Define  $\Delta\mathbf{k} = \mathbf{k}' - \mathbf{k}$  - scattering wave vector

Then  $\Delta\mathbf{k} = \mathbf{G}$ , where  $\mathbf{G}$  is defined as such a vector for which  $\mathbf{G} \cdot \mathbf{T} = 2\pi m$

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We obtained the *diffraction (Laue) condition*:  $\Delta\mathbf{k} = \mathbf{G}$  where  $\mathbf{G} \cdot \mathbf{T} = 2\pi m$

Vectors  $\mathbf{G}$  which satisfy this relation form a *reciprocal lattice*

A reciprocal lattice is defined with reference to a particular Bravais lattice, which is determined by a set of lattice vectors  $\mathbf{T}$ .

### Constricting the reciprocal lattice from the direct lattice:

Let  $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$  - primitive vectors of the direct lattice;  $\mathbf{T} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$

Then reciprocal lattice can be generated using the primitive vectors

$$\mathbf{b}_1 = \frac{2\pi}{V} \mathbf{a}_2 \times \mathbf{a}_3, \quad \mathbf{b}_2 = \frac{2\pi}{V} \mathbf{a}_3 \times \mathbf{a}_1, \quad \mathbf{b}_3 = \frac{2\pi}{V} \mathbf{a}_1 \times \mathbf{a}_2$$

where  $V = \mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)$  is the volume of the unit cell

Then vector  $\mathbf{G} = m_1\mathbf{b}_1 + m_2\mathbf{b}_2 + m_3\mathbf{b}_3$  We have  $\mathbf{b}_i \cdot \mathbf{a}_j = \delta_{ij}$

$$\text{Therefore, } \mathbf{G} \cdot \mathbf{T} = (m_1\mathbf{b}_1 + m_2\mathbf{b}_2 + m_3\mathbf{b}_3) \cdot (n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3) = 2\pi(m_1n_1 + m_2n_2 + m_3n_3) = 2\pi m$$

*The set of reciprocal lattice vectors determines the possible scattering wave vectors for diffraction*

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We got  $\Delta\mathbf{k} = \mathbf{k}' - \mathbf{k} = \mathbf{G} \Rightarrow |\mathbf{k}'|^2 = |\mathbf{k}|^2 + |\mathbf{G}|^2 + 2\mathbf{k}\cdot\mathbf{G} \Rightarrow G^2 + 2\mathbf{k}\cdot\mathbf{G} = 0$

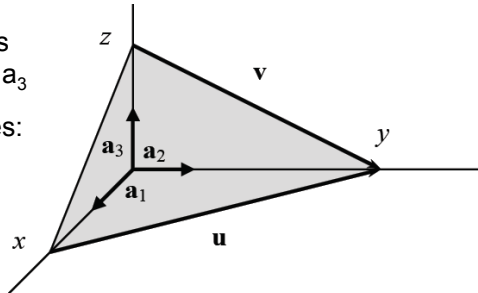
$$2\mathbf{k}\cdot\mathbf{G} = -G^2 \text{ - another expression for diffraction condition}$$

Now, show that the reciprocal lattice vector  $\mathbf{G} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3$  is orthogonal to the plane represented by Miller indices  $(hkl)$

plane  $(hkl)$  intercepts axes at points  $x, y,$  and  $z$  given in units  $a_1, a_2$  and  $a_3$

By the definition of the Miller indices:

$$(h, k, l) = \left( \frac{1}{x}, \frac{1}{y}, \frac{1}{z} \right)$$



define plane by two non-collinear vectors  $\mathbf{u}$  and  $\mathbf{v}$  lying within this plane:

$$\mathbf{u} = ya_2 - xa_1 \text{ and } \mathbf{v} = ya_2 - za_3$$

prove that  $\mathbf{G}$  is orthogonal to  $\mathbf{u}$  and  $\mathbf{v}$ :

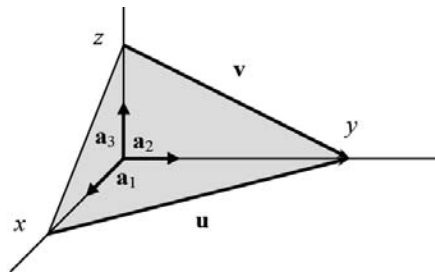
$$\mathbf{u}\cdot\mathbf{G} = (ya_2 - xa_1)\cdot(hb_1 + kb_2 + lb_3) = 2\pi(yk - xh) = 0$$

analogously show

$$\mathbf{v}\cdot\mathbf{G} = 0 \quad 37$$

Now, prove that the distance between two adjacent parallel planes of the direct lattice is  $d = 2\pi/G$ .

The interplanar distance is given by the projection of the one of the vectors  $xa_1, ya_2, za_3,$  to the direction normal to the  $(hkl)$  plane, which is the direction of the unit vector  $\mathbf{G}/G$



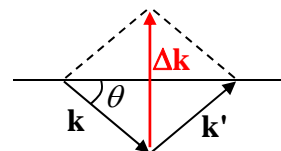
$$\Rightarrow d = xa_1 \cdot \mathbf{G} / G = 2\pi xh / G = 2\pi / G$$

The reciprocal vector  $G(hkl)$  is associated with the crystal planes  $(hkl)$  and is normal to these planes. The separation between these planes is  $2\pi/G$

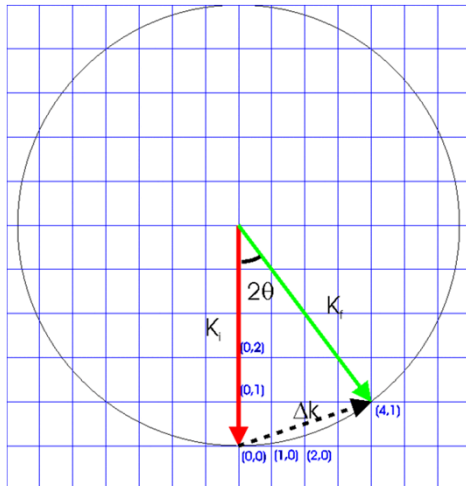
$$2\mathbf{k}\cdot\mathbf{G} = G^2 \Rightarrow 2|\mathbf{k}|G\sin\theta = G^2$$

$$\Rightarrow 2 \cdot 2\pi\sin\theta/\lambda = 2\pi/d \Rightarrow 2d\sin\theta = \lambda$$

$2d\sin\theta = m\lambda$  - get Bragg law



## Ewald Construction for Diffraction Condition and reciprocal space



Diffraction occurs for:

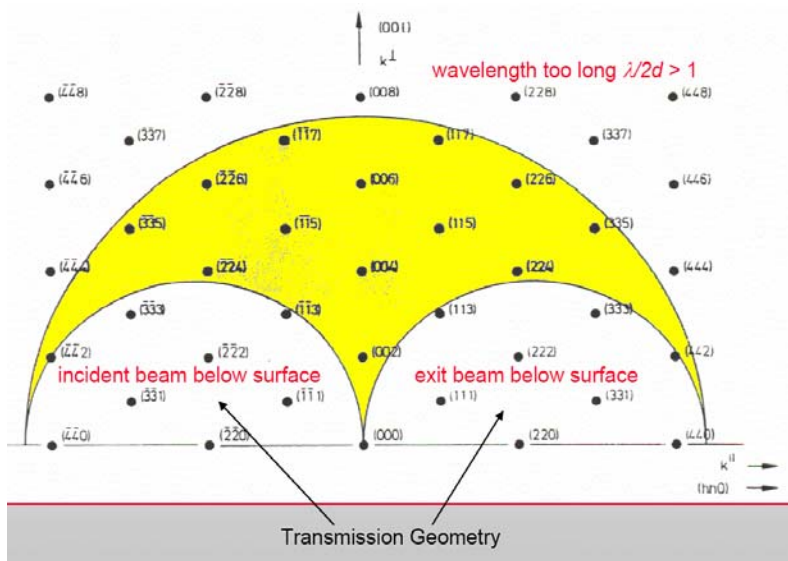
$$\vec{k} + \vec{G} = \vec{k}'$$

Or

$$\vec{k}' - \vec{k} = \vec{G}$$

$$k = 2\pi/\lambda$$

## Reciprocal Space: Accessible Area for Diffraction



### Summary

$$k = 2\pi/\lambda$$

- ❖ Various statements of the Bragg condition:

$$2d \cdot \sin\theta = m\lambda ; \quad \Delta\mathbf{k} = \mathbf{G} ; \quad 2\mathbf{k} \cdot \mathbf{G} = G^2$$

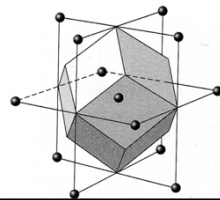
- ❖ Reciprocal lattice is defined by primitive vectors:

$$\mathbf{b}_1 = \frac{2\pi}{V} \mathbf{a}_2 \times \mathbf{a}_3, \quad \mathbf{b}_2 = \frac{2\pi}{V} \mathbf{a}_3 \times \mathbf{a}_1, \quad \mathbf{b}_3 = \frac{2\pi}{V} \mathbf{a}_1 \times \mathbf{a}_2$$

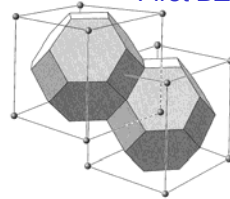
- ❖ A reciprocal lattice vector has the form  $\mathbf{G} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3$   
It is normal to (hkl) planes of direct lattice

- ❖ Only waves whose wave vector drawn from the origin terminates on a surface of the Brillouin zone can be diffracted by the crystal

First BZ of bcc lattice



First BZ of fcc lattice



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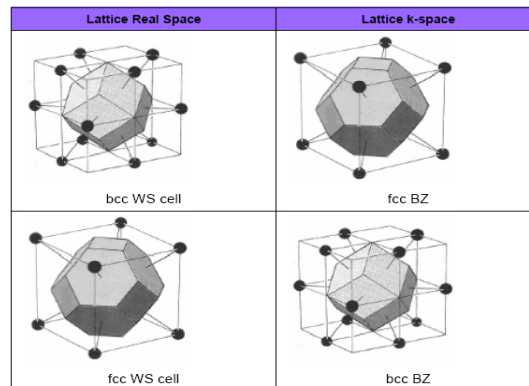
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### Summary

the reciprocal space for a simple cubic lattice is simple cubic, but the other cubic lattice (BCC, FCC) are more confusing:

The BCC and FCC lattices are Fourier transforms of one another



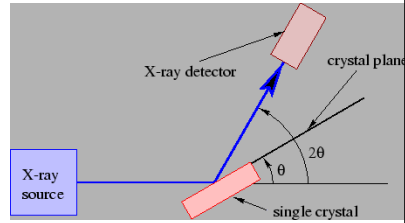
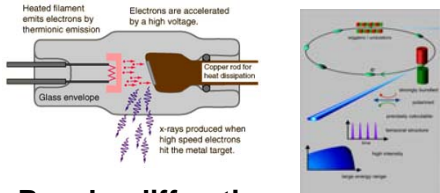
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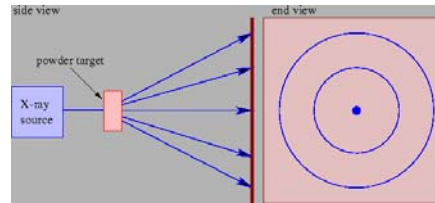
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## Experimental XRD techniques

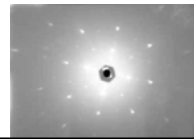
**Rotating crystal method** –  
for single crystals, epitaxial films  
 $\theta$ - $2\theta$ , rocking curve,  $\phi$  - scan



**Powder diffraction**



**Laue method** – *white* x-ray beam most often used for mounting **single** crystals in a precisely known orientation

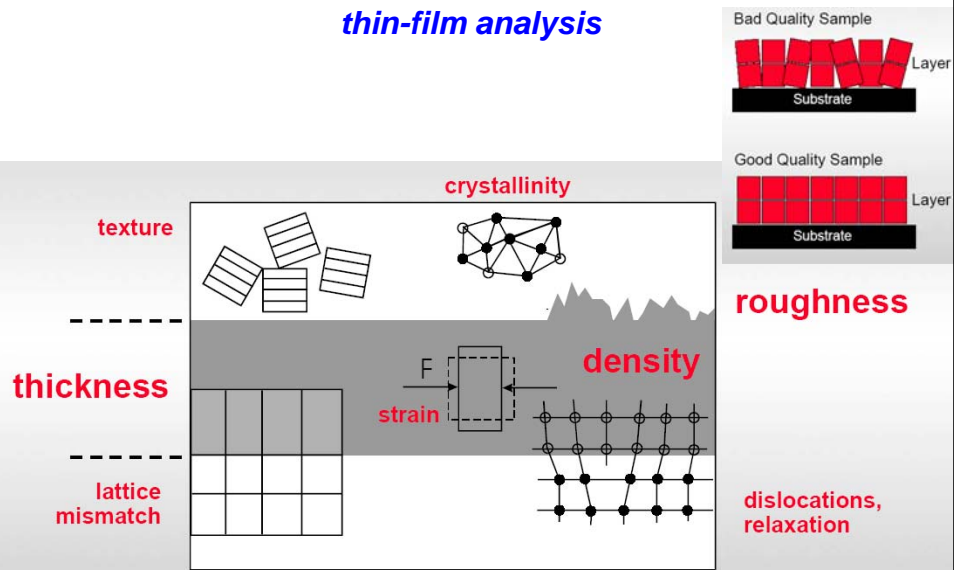


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## Applications of X-ray Diffraction for crystal and thin-film analysis

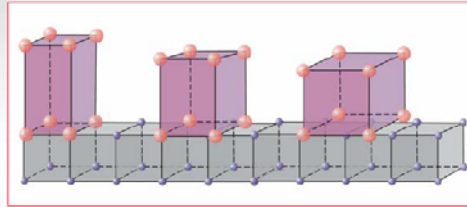
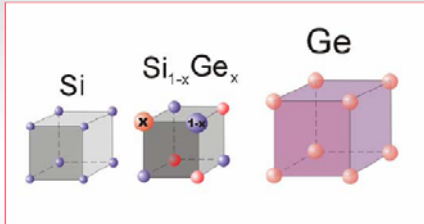


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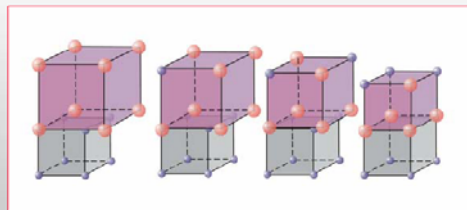
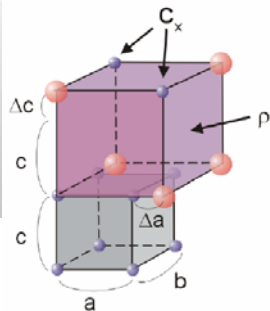
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**Applications of X-ray Diffraction for hetero-structures  
(one or more crystalline films grown on a substrate)**



Relaxation degree

Example:  $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$  structure



Concentration influences lattice constants

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How are diffraction experiments done?

**X-ray Diffraction Setup**



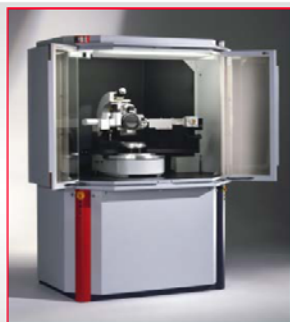
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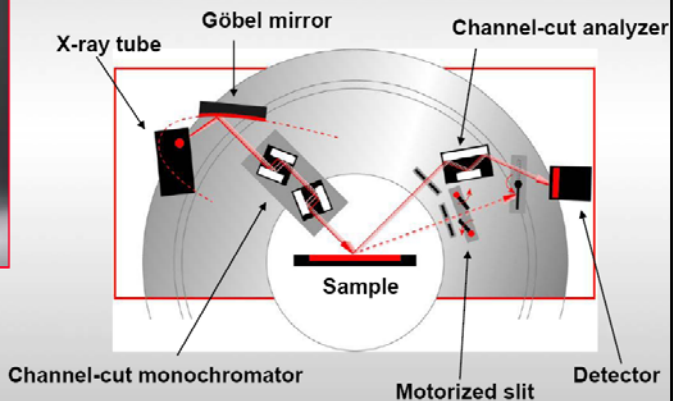
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## High Angular Resolution X-ray Diffraction Setup

B11 Tiernan



D8 Discover

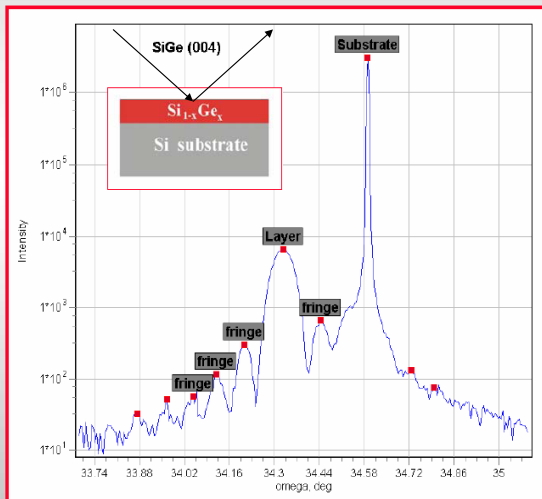


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## Example of High Angular Resolution X-ray Diffraction analysis of a SiGe film on Si substrate



Normal mismatch

$$(\Delta c / c) = (c_L - c_S) / c_S = \frac{\sin \omega_S}{\sin \omega_L} - 1.$$

Assuming  $\Delta a/a = 0$ , Concentration of Ge can be evaluated

Thickness

$$t = \frac{\lambda \sin \omega_e^0}{\sin 2\theta_B |\eta_1 - \eta_2|}; \quad \omega_e^0 = \theta_B + (\pi/2 - \varphi).$$

$$\varphi = \arcsin((\mathbf{h}n/k) / 2 \sin \theta_B)$$

$\eta_{1,2}$  angular deviations of fringes relative to the 0-order layer peak

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